

Why Granular Media Are, After All, Thermal

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Granular media are considered *athermal*, because the grains are too large to display Brownian type thermal fluctuations. On the other hand, being macroscopic, every grain undergoes thermal expansion, possesses a temperature that may be measured with a thermometer, and consists of many, many internal degrees of freedom that in their sum do affect granular dynamics. Therefore, including them in a comprehensive approach to account for granular behavior entails crucial advantages. The pros and cons of thermal versus athermal descriptions are considered.

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Taking grains as athermal particles interacting via the Newtonian law with an elasto-frictional force, discrete element method (DEM) has been a success story [1–3], to the extent that it is today the tool of choice for coming to terms with granular behavior [4]. A second success story is the granular kinetic theory [5–9] that also takes grains as athermal particles colliding with a restitution coefficient smaller than one. As a result – and because granular Brownian motion is imperceptibly small – it is a common place of the granular community that grains may generally be approximated as athermal particles.

This belief is best reflected in athermal statistical mechanics (ASM) that defines, in addition, an entropy S (as the logarithm of the number of grains may be stably packed), assuming it is maximal in equilibrium, if the numbers are appropriately weighted [10–14]. (In contrast, DEM neither needs an entropy to guide the system towards the rest state, nor ever introduces it.) Being non-conserved, energy is typically discarded as a state variable. Instead, S is taken to depend on the volume and force moment tensor. Force equilibrium is often assumed.

This is a leap of faith: Granular Brownian motion is small because grains are macroscopic. But there are then many, many internal microscopic degrees of freedom that one needs to make sure are irrelevant. To see whether they are, consider the textbook example of a pendulum. Its motion is given by the Newtonian force law of a mass point, including a friction term – no need to consider any microscopic degrees here. But to determine the sign of the friction, to make sure that the amplitude diminishes, one needs to consider how the total entropy, consisting mainly of microscopic degrees of freedom, increases. These are the air molecules surrounding the pendulum and the phonons in the string – also the phonons and electrons in the pendular weights, if there are two steel pendula colliding periodically. When the pendula come to a standstill hanging down, their macroscopic energy is zero, and *the total entropy maximal*.

If this is an apt analogy for the relation between DEM and granular statistical mechanics, if the microscopic degrees of freedom do influence the macroscopic dynamics,

they must be included when calculating the entropy.

At any rate, if we consider the air or water surrounding the grains, we need to include their molecular degrees of freedom in an entropic consideration: Is it not consistent to include the inner-granular ones as well?

Doing so, helpfully, the total energy is conserved, and the thermal statistical mechanics valid – as is thermodynamics. Employing them, one finds that the grain-level energy dissipates because it is being redistributed to the microscopic degrees of freedom, and that force equilibrium holds as a result of S being maximal.

We therefore submit: *Granular media are not generally athermal. More specifically, taking a reduced entropy that excludes internal degrees of freedom as maximal in equilibrium, one bears a heavy burden of proof.*

Two-stage irreversibility, a useful notion for coming to terms with granular thermodynamics is related to the three spatial scales of any granular media: (a) the macroscopic, (b) the mesoscopic or inter-granular, and (c) the microscopic or inner granular. Dividing all degrees of freedom into these three categories, one treats those of (a) differently from (b,c). Macroscopic degrees of freedom (the slowly varying stress, flow and density fields) are employed as state variables, but inter- and inner granular degrees of freedom are treated summarily: Only their contributions to the energy are considered and taken, respectively, as granular and true heat. One does not account for the microscopic dynamics of phonons and electrons, but takes the sum of their energy as $\int T dS$. Similarly, one does not account for the motion and deformation of every grain, only includes their fluctuating kinetic and elastic energy as granular heat W_T . Defining S_g as the logarithm of the number of states the inter-granular degrees may be in, and $T_g \equiv \partial W_T / \partial S_g$, we again have $W_T = \int T_g dS_g$. There are a handful of macroscopic degrees of freedom (a), a large number of inter-granular ones (b), and yet many orders of magnitude more inner granular ones (c). So the statistical tendency to equally distribute the energy among all degrees of freedom implies an energy decay: (a \rightarrow c) and (a \rightarrow b \rightarrow c), or what

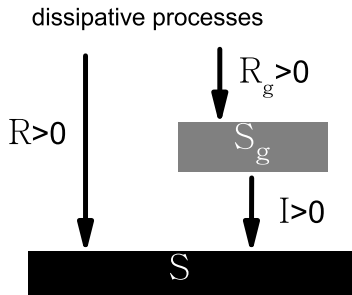


FIG. 1. Dissipative processes produce either granular entropy S_g , or thermal entropy S . Eventually, S_g also decays to S . Irreversibility is implied by the three energy-decay terms R , R_g , I being always positive. Containing all states of deformed and moving grains, S_g is a much larger quantity than various versions of the reduced entropy in ASM, though $S_g \ll S$ still holds. The system is in equilibrium if $S_{tot} \equiv S + S_g \approx S$ is maximal. Maximal S_g characterizes (quasi-)equilibrium for times $t \ll \tau$ (with τ the time scale of I). Then conventional statistical mechanics and thermodynamics hold. Maximal S_g for $t \rightarrow \infty$ is a novel proposition.

we termed *two-stage irreversibility*, see Fig 1.

Starting from two-stage irreversibility and the resultant granular thermodynamics, a hydrodynamic theory for granular media (named GSH for “granular solid hydrodynamics”) was derived [15–18], and it has proven capable of accounting for a wide range of granular phenomena, including (i) static stress distribution, clogging; (ii) elasto-plastic motion: loading and unloading, approach to the critical state, angle of stability and repose; (iii) rapid dense flow: the μ -rheology, Bagnold scaling and the stress minimum; (iv) elastic waves, compaction, wide and narrow shear band; (v) the less conventional experiments of shear jamming, creep flow, visco-elastic behavior and nonlocal fluidization [19].

A division into three scales works well when they are clearly separated – though this is a problem of accuracy, not viability. Scale separation is well satisfied in large-scaled, engineering-type experiments, but less so in small-scaled ones. Using glass or steel beads aggravates the problem. The same is true of 2D experiments employing less and larger disks. On the other hand, when there is too little space for spatial averaging, one may still average over time and runs, to get rid of fluctuations not contained in a hydrodynamic theory.

The fluctuation-dissipation theorem (FDT) correlates the thermal fluctuations of the microscopic degrees of freedom in equilibrium to how they return to equilibrium after having been exposed to a small applied perturbation, ie., to the friction and dissipation that they experience [20]. The microscopic degrees of freedom are atoms or molecules in gas and liquid, and phonons, free electrons in solid. So there is no reason why FDT, a general principle, should not be valid in granular media: FDT holds in a block of copper, although it is much larger

than a grain and has even smaller Brownian motion. This remains so when one cuts the block in half, because a cut is too small and macroscopic a perturbation to appreciably affect FDT, or the linear response theory employed to deduce it. Further cuts are also allowed, as long as the pieces remain macroscopic. The link between thermal fluctuations and the return to equilibrium will not be severed – although the link may change, because the system’s hydrodynamics (such as given by GSH) does. This conclusion clearly holds for all granular media.

The alleged problem with FDT lies elsewhere: Due to random packaging, grains as such also fluctuate – with respect to their position, velocity and external forces. Although these grain-level, non-thermal fluctuations are much stronger and the ones being observed, there is, *prima facie*, no general principle linking them to dissipation. Still, attempts abound to find a T from these fluctuations such that FDT does hold, see [13, 14, 21]. There are many observations on whether FDT is valid, experimental and numerical, and the considered link is always to grain-level fluctuations: Thermal fluctuations are universally set to zero in DEM, and it is difficult, if at all possible, to separate both in experiments.

The Onsager relation (OR) is a direct consequence of FDT. If the latter holds, so does the former. But there is also an independent counter-argument that we need to deal with: The validity of the OR depends on the *time reversal invariance* of the underlying microscopic dynamics, yet grains collide inelastically and execute irreversible motion. This is why many believe OR need not hold in granular media, see [22]. This point of view again ignores the fact that grains are not elementary. The granular kinetic theory is a truncated one, and the apparent lack of time reversal symmetry is a result of this truncation. The microscopic degrees of freedom in sand obey, as everywhere else, the *reversible* Schrödinger equation.

OR concerns the pairwise equality (with same or opposite signs) of transport coefficients, a fact that may be verified experimentally. Although no one is capable of employing the Schrödinger equation to calculate the coefficients directly, there should be little doubt that the result will comply with the OR. Therefore, a proper calculation employing the dissipative kinetic theory must arrive at the same result. (This may not be easy, as the kinetic theory at present only considers R_g , not R , see Fig 1.) More generally, OR is valid in all condensed systems: solids, superfluids, liquid crystals, because all share the same microscopic dynamics. Breaking a solid block into (macroscopic) pieces does not change this fact.

Is T_g a true temperature? Yes, T_g and T each characterizes the energy of a group of degrees of freedom, with a given rate of energy transfer between them. Usually, the degrees of freedom of two systems in thermal contact are spatially separated. In this case, they are not, which

is the main difference. Any difficulties treating T_g as a temperature arise because one ignores T – as in the cases discussed above, and it is also the reason for the failure of granular media to equilibrate, that granular temperatures of two systems in contact are different.

Given two granular systems, 1 and 2, with only 1 being excited, there are, in the steady state, four generally unequal temperatures: T^1, T_g^1, T^2, T_g^2 , and an ongoing energy transfer ($T_g^1 \rightarrow T^1$), ($T_g^1 \rightarrow T_g^2$) and ($T_g^2 \rightarrow T^2$). Their differences depend on details such as the restitution coefficients and the contact area. This is quite similar to four thermal systems, two large (1, 2), two small (1a, 2a), with (1a) being heated, and (1a, 1), (1a, 2a), (2a, 2) in pairwise thermal contact. All four temperatures will usually be different, and there is an ongoing energy flux.

The passive granular system 2 may serve as a thermometer if it consisted of completely elastic beads, and if both are separated by a massless membrane that transmits momentum but no particles. (So this is more a DEM-thermometer.) In the steady state, we have $T_g^1 = T_g^2$, and the energy transfer ($T_g^1 \rightarrow T_g^2$) vanishes. Similarly, if system 2 does not exist, we have $T_a^1 = T_a^2$.

Finally, a caveat: Employing T_g to quantify the granular degrees of freedom is sensible only if these are in *equilibrium with one another*. This is not always the case, eg. a granular gas maintained by vibrating walls, which therefore needs additional state variables, see [23]. But grains become increasingly better equilibrated for higher densities and longer lasting contacts. To keep the discussion simple, we assume here that they are.

Granular Thermodynamics has, as its set of state variables, first the usual ones: the density ρ , the momentum density ρv_i , the total entropy s_{tot} ; then in addition: the granular entropy s_g , the elastic strain u_{ij} . (The elastic strain u_{ij} is a coarse-grained measure of the grains' elastic deformation, and not the total strain, see [15–17].) Denoting the conserved energy density (in the rest frame, $v_i = 0$) as $w = w(s, s_g, \rho, u_{ij})$, the conjugate variables are: $T \equiv \partial w / \partial s$, $T_g \equiv \partial w / \partial s_g$, $\mu \equiv \partial w / \partial \rho$, $\pi_{ij} \equiv -\partial w / \partial u_{ij}$, where μ is the chemical potential and π_{ij} the elastic stress. This is conveniently written as

$$dw = Tds + T_g ds_g + \mu d\rho - \pi_{ij} du_{ij}, \quad (1)$$

a formula valid as long as the variables are as given. Writing $Tds + T_g ds_g = Td(s + s_g) + (T_g - T)ds_g$, we identify the first term as the equilibrium energy for $T_g = T$, and the second as the additional contribution if $T_g \neq T$. Characterizing the non-optimal energy distribution between the inter- and inner granular degrees of freedom, $T_g - T$ relaxes until it vanishes. Now, since $s \gg s_g$, and since any granular motion at all already implies $T_g \gg T$, we have $T_g - T \approx T_g$, $s + s_g \approx s$, and this rewriting does not change anything. So we may take T_g as the relaxing quantity, with $T_g = 0$ replacing $T_g = T$ at equilibrium. [This result is essential for obtaining Eq.(4).]

Formal equilibrium conditions, given in terms of the conjugate variables and valid irrespective what the actual expression for $w = w(s, s_g, \rho, u_{ij})$ is, are obtained by requiring $\int s d^3r$ to be maximal, under the constraints of constant energy $\int w d^3r$ and mass $\int \rho d^3r$. In granular media, remarkably, this universally valid procedure leads to two sets of equilibrium conditions, solid- and fluid-like.

Maximizing the entropy (see [15–17] for details), we always obtain $\nabla_i T = 0$, and $T_g = 0$. Usually, T_g vanishes quickly, and if it does, the density no longer varies independently from the elastic strain, $d\rho/\rho = -du_{\ell\ell}$. They then share a common, solid-like equilibrium condition,

$$\nabla_i(\pi_{ij} + P_T \delta_{ij}) = \rho g_i, \quad (2)$$

where g_i is the gravitational constant, π_{ij} the elastic stress, $P_T \equiv -\partial(wV)/\partial V$ the usual fluid pressure (V is the volume, and the derivative is taken at constant ρV , $s_{tot}V$ and $s_g V$). With Eq.(4) below, $P_T \sim T_g^2 \rightarrow 0$ is the pressure exerted by jiggling grains. Clearly, Eq (2) expresses force balance in the jammed state.

If T_g is kept finite by continual external perturbations, the system further increases its entropy by independently varying ρ and u_{ij} , to arrive at the fluid equilibrium, characterized by two conditions. The first, with respect to u_{ij} , requires any shear stress to vanish and any free surface to be horizontal in equilibrium; the second is related to reversible compaction, see [19] for more details:

$$\pi_{ij} = 0, \quad \nabla_i P_T = \rho g_i. \quad (3)$$

The relation between T_g and S_g : In the gaseous phase, grains have only kinetic energy, $\frac{1}{2}T_g$ per degree of freedom. With N the number of grains, the total energy is $W_T = \frac{3}{2}T_g N$. If the inner granular degrees of freedom may be modeled as a phonon gas, the inner energy is $3TN_a$ (for $T \gg T_D$, the Debye temperature, and with N_a the number of atoms in all the grains). Assuming (unrealistically) that the grains maintained their integrity at arbitrarily high T , they will heat up during a collision for $T_g > T$, but cool down for $T_g < T$, until $T_g = T$, a result associated with the total energy being conserved. Usually, of course, because $T_g \gg T$, the heat transfer is accounted for by a constant restitution coefficient.

This picture becomes blurred at higher densities, breaking down completely when the contacts are enduring. Given the friction between grains, a suitable $w(s_g)$ is difficult to obtain microscopically. Therefore, we pragmatically expand w in s_g , requiring $T_g = 0$ to be minimal. Denoting $w_T = w - w(T_g = 0)$, we have

$$w_T = s_g^2 / 2\rho b = \rho b T_g^2 / 2, \quad T_g \equiv \partial w / \partial s_g|_s = s_g / \rho b. \quad (4)$$

As this expression assumes only analyticity of w and does not depend on interactions, it is quite general – as long as T_g is sufficiently small.

One could now find an appropriate formula interpolating between this limit and the gaseous one. But we,

rather more simply, employ Eq.(4) for all values of T_g . This works because of T_g 's two functions, as a measure for equilibration and as a state variable, only the second is relevant in praxise: Substituting $w_T = \rho b T_g^2/2$ for $w_T = \frac{3}{2} T_k \rho/m$ implies $T_k = \frac{1}{3} m b T_g^2$ in the gaseous limit (m is the average mass of a grain, T_k is introduced to distinguish both). This is impermissible when one considers equilibration, as done above, because it is T_k that becomes equal to T , not T_g . On the other hand, such super hot grains do not exist, and equilibration (though helpful for coming to terms with T_g) is not a realistic scenario. The second, and relevant, role of T_g does not possess such a scale. For instance, the pressure is found $\sim T_k$, the viscosity $\sim \sqrt{T_k}$, in the kinetic theory and in DEM, see [24, 25], while they are, respectively, $\sim T_g^2$ and $\sim T_g$ in GSH. So Eq.(4) may be taken as valid throughout, and in fact defines T_g .

Conclusions: Given the three length scales in any granular media: macroscopic, granular and microscopic, two temperatures: T, T_g are relevant, and the entropy is the sum of all granular and microscopic degrees of freedom. Thermodynamics holds, and T_g is well-behaved, if one includes T in all considerations. A jammed state at rest is in equilibrium, with the entropy being maximal. Fluctuation-dissipation theorem, correlating dissipation to thermal fluctuations, holds in granular media as in any other system. The strong, nonthermal grain-level stochasticity – such as force chains, or stick and slip motion – has yet to find a theory. But the macroscopic granular dynamics, averaged over thermal and grain-level fluctuations, is well accounted for by GSH.

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